Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2017 – 03:21 am GMT

PDB ID	:	5EFZ
Title	:	Monoclinic structure of the acetyl esterase MekB
Authors	:	Toelzer, C.; Pal, S.; Watzlawick, H.; Altenbuchner, J.; Niefind, K.
Deposited on	:	2015-10-26
Resolution	:	1.82 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

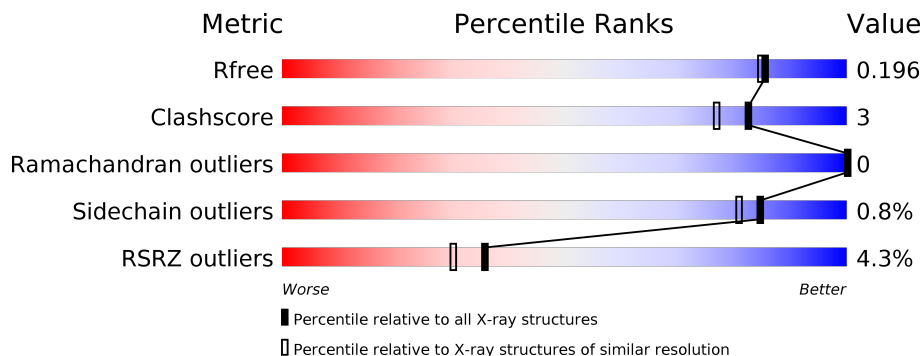|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.196
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0.8%
RSRZ outliers		4.3%

Worse — Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	100719	5868 (1.84-1.80)
Clashscore	112137	6856 (1.84-1.80)
Ramachandran outliers	110173	6780 (1.84-1.80)
Sidechain outliers	110143	6780 (1.84-1.80)
RSRZ outliers	101464	5947 (1.84-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	361	91% 5% •
1	B	361	90% 6% •
1	C	361	90% • 6%
1	D	361	13% / 87% 9% •
1	E	361	10% / 87% 8% •
1	F	361	93% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	401	-	-	-	X
2	EDO	A	403	-	-	-	X
2	EDO	A	405	-	-	-	X
2	EDO	A	406	-	-	-	X
2	EDO	A	407	-	-	-	X
2	EDO	B	403	-	-	-	X
2	EDO	B	404	-	-	-	X
2	EDO	C	401	-	-	-	X
2	EDO	C	402	-	-	-	X
2	EDO	C	403	-	-	-	X
2	EDO	C	404	-	-	X	X
2	EDO	C	406	-	-	-	X
2	EDO	D	401	-	-	X	-
2	EDO	D	403	-	-	-	X
2	EDO	E	402	-	-	-	X
2	EDO	F	401	-	-	-	X
3	GOL	A	408	-	-	-	X
3	GOL	C	408	-	-	-	X
3	GOL	F	403	-	-	-	X
3	GOL	F	404	-	-	-	X
3	GOL	F	405	-	-	-	X
4	ACT	C	409	-	-	-	X
4	ACT	D	406	-	-	-	X
4	ACT	E	404	-	-	-	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 17233 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Homoserine O-acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	2	0
			2693	1709	459	509	16			
1	B	345	Total	C	N	O	S	0	2	0
			2678	1699	458	505	16			
1	C	339	Total	C	N	O	S	0	0	0
			2602	1653	448	485	16			
1	D	345	Total	C	N	O	S	0	0	0
			2661	1688	456	501	16			
1	E	345	Total	C	N	O	S	0	0	0
			2660	1689	455	500	16			
1	F	347	Total	C	N	O	S	0	0	0
			2678	1701	457	504	16			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q0MRG5
A	-10	THR	-	expression tag	UNP Q0MRG5
A	-9	MET	-	expression tag	UNP Q0MRG5
A	-8	ILE	-	expression tag	UNP Q0MRG5
A	-7	THR	-	expression tag	UNP Q0MRG5
A	-6	HIS	-	expression tag	UNP Q0MRG5
A	-5	HIS	-	expression tag	UNP Q0MRG5
A	-4	HIS	-	expression tag	UNP Q0MRG5
A	-3	HIS	-	expression tag	UNP Q0MRG5
A	-2	HIS	-	expression tag	UNP Q0MRG5
A	-1	HIS	-	expression tag	UNP Q0MRG5
A	0	GLY	-	expression tag	UNP Q0MRG5
A	1	SER	-	expression tag	UNP Q0MRG5
B	-11	MET	-	initiating methionine	UNP Q0MRG5
B	-10	THR	-	expression tag	UNP Q0MRG5
B	-9	MET	-	expression tag	UNP Q0MRG5
B	-8	ILE	-	expression tag	UNP Q0MRG5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	THR	-	expression tag	UNP Q0MRG5
B	-6	HIS	-	expression tag	UNP Q0MRG5
B	-5	HIS	-	expression tag	UNP Q0MRG5
B	-4	HIS	-	expression tag	UNP Q0MRG5
B	-3	HIS	-	expression tag	UNP Q0MRG5
B	-2	HIS	-	expression tag	UNP Q0MRG5
B	-1	HIS	-	expression tag	UNP Q0MRG5
B	0	GLY	-	expression tag	UNP Q0MRG5
B	1	SER	-	expression tag	UNP Q0MRG5
C	-11	MET	-	initiating methionine	UNP Q0MRG5
C	-10	THR	-	expression tag	UNP Q0MRG5
C	-9	MET	-	expression tag	UNP Q0MRG5
C	-8	ILE	-	expression tag	UNP Q0MRG5
C	-7	THR	-	expression tag	UNP Q0MRG5
C	-6	HIS	-	expression tag	UNP Q0MRG5
C	-5	HIS	-	expression tag	UNP Q0MRG5
C	-4	HIS	-	expression tag	UNP Q0MRG5
C	-3	HIS	-	expression tag	UNP Q0MRG5
C	-2	HIS	-	expression tag	UNP Q0MRG5
C	-1	HIS	-	expression tag	UNP Q0MRG5
C	0	GLY	-	expression tag	UNP Q0MRG5
C	1	SER	-	expression tag	UNP Q0MRG5
D	-11	MET	-	initiating methionine	UNP Q0MRG5
D	-10	THR	-	expression tag	UNP Q0MRG5
D	-9	MET	-	expression tag	UNP Q0MRG5
D	-8	ILE	-	expression tag	UNP Q0MRG5
D	-7	THR	-	expression tag	UNP Q0MRG5
D	-6	HIS	-	expression tag	UNP Q0MRG5
D	-5	HIS	-	expression tag	UNP Q0MRG5
D	-4	HIS	-	expression tag	UNP Q0MRG5
D	-3	HIS	-	expression tag	UNP Q0MRG5
D	-2	HIS	-	expression tag	UNP Q0MRG5
D	-1	HIS	-	expression tag	UNP Q0MRG5
D	0	GLY	-	expression tag	UNP Q0MRG5
D	1	SER	-	expression tag	UNP Q0MRG5
E	-11	MET	-	initiating methionine	UNP Q0MRG5
E	-10	THR	-	expression tag	UNP Q0MRG5
E	-9	MET	-	expression tag	UNP Q0MRG5
E	-8	ILE	-	expression tag	UNP Q0MRG5
E	-7	THR	-	expression tag	UNP Q0MRG5
E	-6	HIS	-	expression tag	UNP Q0MRG5
E	-5	HIS	-	expression tag	UNP Q0MRG5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP Q0MRG5
E	-3	HIS	-	expression tag	UNP Q0MRG5
E	-2	HIS	-	expression tag	UNP Q0MRG5
E	-1	HIS	-	expression tag	UNP Q0MRG5
E	0	GLY	-	expression tag	UNP Q0MRG5
E	1	SER	-	expression tag	UNP Q0MRG5
F	-11	MET	-	initiating methionine	UNP Q0MRG5
F	-10	THR	-	expression tag	UNP Q0MRG5
F	-9	MET	-	expression tag	UNP Q0MRG5
F	-8	ILE	-	expression tag	UNP Q0MRG5
F	-7	THR	-	expression tag	UNP Q0MRG5
F	-6	HIS	-	expression tag	UNP Q0MRG5
F	-5	HIS	-	expression tag	UNP Q0MRG5
F	-4	HIS	-	expression tag	UNP Q0MRG5
F	-3	HIS	-	expression tag	UNP Q0MRG5
F	-2	HIS	-	expression tag	UNP Q0MRG5
F	-1	HIS	-	expression tag	UNP Q0MRG5
F	0	GLY	-	expression tag	UNP Q0MRG5
F	1	SER	-	expression tag	UNP Q0MRG5

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	E	1	Total 4	C 2	O 2	0	0
2	E	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total 4	C 2	O 2	0	0
2	F	1	Total 4	C 2	O 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
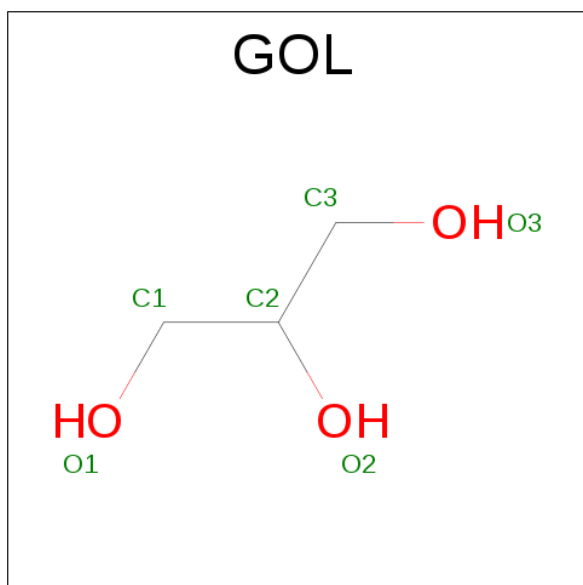
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	F	1	Total 6	C 3	O 3	0	0
3	F	1	Total 6	C 3	O 3	0	0
3	F	1	Total 6	C 3	O 3	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
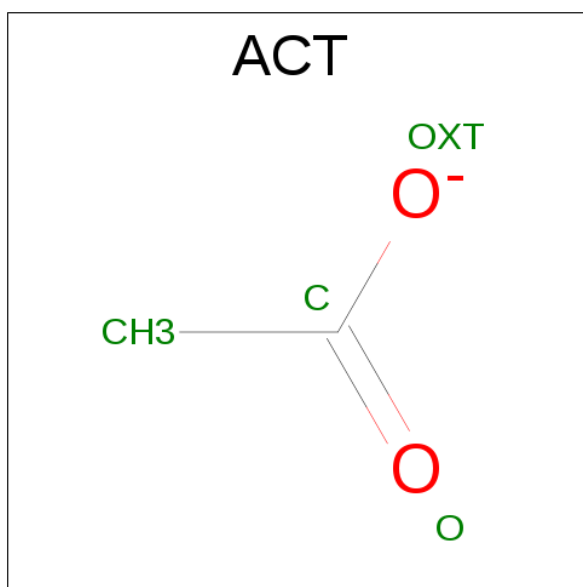
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	F	1	Total 4	C 2	O 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	213	Total 213	O 213	0	0
5	B	207	Total 207	O 207	0	0
5	C	181	Total 181	O 181	0	0
5	D	124	Total 124	O 124	0	0
5	E	119	Total 119	O 119	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	241	Total 241	O 241	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
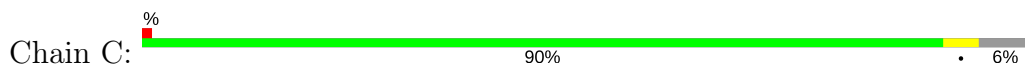
- Molecule 1: Homoserine O-acetyltransferase

- Molecule 1: Homoserine O-acetyltransferase

- Molecule 1: Homoserine O-acetyltransferase

- Molecule 1: Homoserine O-acetyltransferase

- Molecule 1: Homoserine O-acetyltransferase

Chain E:

10%

87%

8%

MET THR MET ILE THR HIS HIS HIS HIS HIS HIS GLY SER ASN S3 Y4 Y5 T6 E7 E8 N9 H10 G11 P12 F13 E14 L23 R27 C28 M29 H39 G40 A41 L42 N43 A44 D45 K46 S47 W55 E64 I68 G69 E70 G71 G106 E125 Y126 F127 G128 I129 E130

S139 R151 Y152 K157 E181 R195 E205 T212 E219 F220 F221 R222 R225 G230 F231 E232 Q235 M236 D239 G240 F241 M242 K243 R244 F295 H322 P347 ALA TYR

• Molecule 1: Homoserine O-acetyltransferase

Chain F:

93%

MET THR MET ILE THR HIS HIS HIS HIS HIS HIS GLY SER ASN S3 N17 E24 E31 H39 W55 E64 D114 L132 V135 I180 L210 P218 L255 Y349
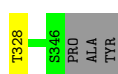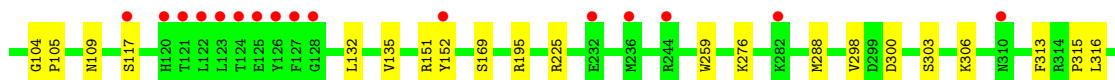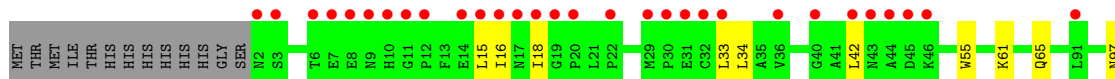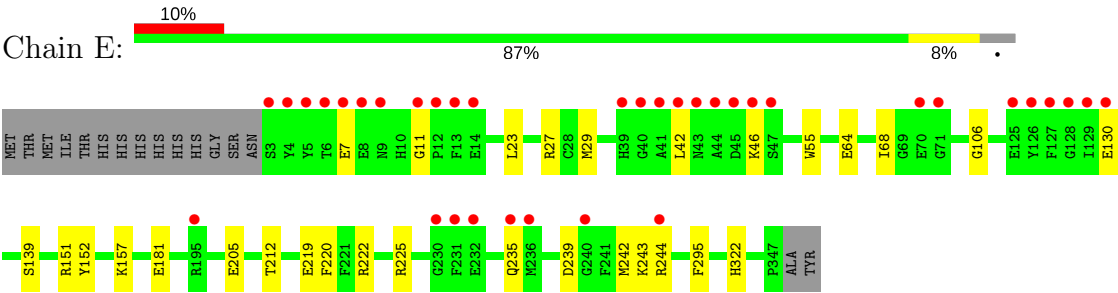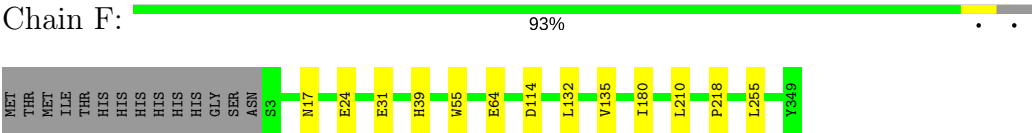
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.85Å 110.34Å 122.82Å 90.00° 106.89° 90.00°	Depositor
Resolution (Å)	46.28 – 1.82 46.28 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.28-1.82) 99.6 (46.28-1.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 1.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.163 , 0.196 0.163 , 0.196	Depositor DCC
R_{free} test set	2138 reflections (1.06%)	DCC
Wilson B-factor (Å^2)	22.6	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 61.8	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	17233	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, EDO, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.60	0/2759	0.61	1/3739 (0.0%)
1	B	0.57	0/2743	0.61	0/3718
1	C	0.53	0/2665	0.58	0/3612
1	D	0.48	0/2725	0.59	0/3693
1	E	0.45	0/2725	0.54	0/3694
1	F	0.62	0/2744	0.62	0/3719
All	All	0.55	0/16361	0.59	1/22175 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	MET	CG-SD-CE	-5.78	90.95	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2693	0	2611	14	0
1	B	2678	0	2600	18	0
1	C	2602	0	2545	11	0
1	D	2661	0	2587	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2660	0	2588	18	0
1	F	2678	0	2602	7	0
2	A	28	0	42	3	0
2	B	20	0	30	3	0
2	C	24	0	36	6	0
2	D	12	0	18	7	0
2	E	8	0	12	0	0
2	F	8	0	12	0	0
3	A	6	0	8	1	0
3	C	12	0	16	2	0
3	D	12	0	16	1	0
3	F	18	0	24	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
4	C	4	0	3	0	0
4	D	4	0	3	0	0
4	E	8	0	6	1	0
4	F	4	0	3	0	0
5	A	213	0	0	1	0
5	B	207	0	0	4	0
5	C	181	0	0	1	0
5	D	124	0	0	3	0
5	E	119	0	0	0	0
5	F	241	0	0	0	0
All	All	17233	0	15768	93	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (93) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:LYS:HG3	1:D:65:GLN:HE22	1.38	0.87
1:B:263:ARG:HE	2:B:405:EDO:H11	1.45	0.81
1:D:195:ARG:NH1	5:D:502:HOH:O	2.15	0.79
1:D:300:ASP:OD2	2:D:401:EDO:H22	1.85	0.77
1:D:151:ARG:NH1	1:D:152:TYR:OH	2.23	0.72
1:E:42:LEU:HD13	1:E:46:LYS:HD2	1.72	0.70
1:D:61:LYS:HG3	1:D:65:GLN:NE2	2.06	0.70
1:B:288:MET:HE1	1:B:339:HIS:HB3	1.74	0.69
1:D:169:SER:OG	2:D:401:EDO:H21	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ASN:H	2:C:404:EDO:H12	1.59	0.68
1:C:109:ASN:H	2:C:404:EDO:C1	2.08	0.67
1:D:15:LEU:HD21	1:D:33:LEU:HB3	1.78	0.66
2:D:401:EDO:O1	5:D:501:HOH:O	2.11	0.64
1:C:273:ASP:CG	1:C:276:LYS:HG3	2.21	0.61
1:A:234:MET:HG3	1:B:170:GLU:HB3	1.82	0.61
3:C:408:GOL:H32	1:D:298:VAL:HG11	1.84	0.59
1:C:185:THR:HG23	1:C:206:ARG:NH2	2.18	0.59
1:D:306:LYS:NZ	2:D:402:EDO:H21	2.19	0.57
1:B:280:ARG:HD3	5:B:513:HOH:O	2.06	0.56
1:C:199:ALA:HB2	3:C:408:GOL:H2	1.88	0.56
1:C:209:LYS:NZ	1:E:181:GLU:OE2	2.37	0.55
1:D:18:ILE:HD11	1:D:34:LEU:HD11	1.88	0.54
1:C:27:ARG:HD2	2:C:404:EDO:H22	1.89	0.54
1:D:169:SER:CB	2:D:401:EDO:H21	2.38	0.54
1:D:151:ARG:HD3	1:D:152:TYR:CE2	2.43	0.54
1:E:205:GLU:HG2	1:E:243:LYS:HE3	1.89	0.54
3:D:405:GOL:H12	1:F:210:LEU:HD11	1.90	0.53
1:E:27:ARG:NH1	1:E:106:GLY:O	2.43	0.52
1:D:15:LEU:HD11	1:D:33:LEU:CG	2.39	0.52
1:B:263:ARG:HH21	2:B:405:EDO:H21	1.73	0.52
1:B:294[B]:GLN:NE2	5:B:503:HOH:O	2.42	0.52
1:B:39:HIS:NE2	1:B:64[A]:GLU:HG2	2.25	0.51
1:F:17:ASN:HD21	1:F:31:GLU:CD	2.14	0.51
1:C:185:THR:HG23	1:C:206:ARG:HH21	1.76	0.51
1:A:234:MET:CE	1:B:174:LEU:HB2	2.41	0.50
1:B:206:ARG:NH1	5:B:502:HOH:O	2.28	0.50
1:F:24:GLU:HG3	1:F:114:ASP:OD1	2.12	0.49
2:D:401:EDO:H12	1:F:218:PRO:HB3	1.95	0.49
1:A:7:GLU:OE1	1:A:12:PRO:HA	2.13	0.48
1:B:263:ARG:HH21	2:B:405:EDO:C2	2.26	0.48
1:B:288:MET:HE3	1:B:314:ARG:HB2	1.95	0.48
1:F:180:ILE:HG23	1:F:255:LEU:HD22	1.95	0.48
1:A:158:ARG:HH22	2:A:403:EDO:H11	1.79	0.48
1:D:225:ARG:NH2	1:D:328:THR:O	2.38	0.48
1:E:23:LEU:HD11	1:E:29:MET:HG3	1.95	0.48
2:C:403:EDO:H21	5:C:546:HOH:O	2.13	0.47
1:D:15:LEU:HD13	1:D:16:ILE:N	2.29	0.47
1:E:219:GLU:OE2	1:E:222:ARG:NH2	2.38	0.47
1:D:303:SER:HA	2:D:402:EDO:H22	1.97	0.47
1:E:220:PHE:CE2	1:E:225:ARG:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLY:HA2	1:A:162:ILE:O	2.14	0.47
1:E:151:ARG:HD3	1:E:152:TYR:CE1	2.50	0.47
1:D:97:ASN:HB3	5:D:517:HOH:O	2.15	0.47
1:E:157:LYS:HA	1:E:157:LYS:HD3	1.73	0.46
1:D:117:SER:HB2	1:D:151:ARG:NH2	2.31	0.46
1:E:235:GLN:NE2	1:E:239:ASP:OD2	2.48	0.46
1:E:212:THR:OG1	1:E:242:MET:HG3	2.16	0.46
1:C:107:PHE:HB3	2:C:403:EDO:H21	1.99	0.45
1:D:276:LYS:HE3	1:D:276:LYS:HB2	1.70	0.45
1:B:132:LEU:HD13	1:B:135:VAL:HG22	1.98	0.45
1:E:139:SER:OG	4:E:403:ACT:OXT	2.32	0.45
1:B:64[A]:GLU:HA	1:B:68:ILE:HD12	1.98	0.45
1:A:262:GLN:O	2:A:405:EDO:H11	2.17	0.45
1:C:109:ASN:H	2:C:404:EDO:H11	1.80	0.45
1:D:15:LEU:HD11	1:D:33:LEU:HG	1.99	0.45
1:D:15:LEU:C	1:D:15:LEU:HD13	2.37	0.45
1:C:313:PHE:CE2	1:C:315:PRO:HG3	2.51	0.44
1:D:15:LEU:HD11	1:D:33:LEU:HB3	1.98	0.44
1:E:64:GLU:HA	1:E:68:ILE:HD12	1.99	0.44
1:F:132:LEU:HD13	1:F:135:VAL:HG22	1.98	0.44
1:A:24[B]:GLU:OE2	1:A:151:ARG:NH2	2.41	0.44
1:A:158:ARG:HH12	2:A:403:EDO:H12	1.82	0.44
1:B:64[B]:GLU:HA	1:B:68:ILE:HD12	1.99	0.44
1:A:180:ILE:HG23	1:A:255:LEU:HD22	2.01	0.43
1:A:288:MET:HE2	1:A:316:LEU:HD21	2.00	0.43
1:B:180:ILE:HG23	1:B:255:LEU:HD22	2.00	0.43
1:E:220:PHE:CD2	1:E:225:ARG:HG2	2.53	0.43
1:E:295:PHE:HZ	1:E:322:HIS:CD2	2.35	0.43
1:A:3:SER:N	5:A:506:HOH:O	2.51	0.42
1:B:24:GLU:HG3	1:B:114:ASP:OD1	2.18	0.42
1:D:313:PHE:CE2	1:D:315:PRO:HG3	2.54	0.42
1:E:295:PHE:CZ	1:E:322:HIS:CD2	3.07	0.42
1:D:132:LEU:HD13	1:D:135:VAL:HG22	2.00	0.42
1:A:24[A]:GLU:OE2	1:A:268:ARG:NH2	2.50	0.42
1:A:188:ALA:HA	3:A:408:GOL:H12	2.01	0.42
1:F:39:HIS:NE2	1:F:64:GLU:HG2	2.35	0.41
1:D:288:MET:CE	1:D:316:LEU:HD21	2.51	0.41
1:B:3:SER:N	5:B:514:HOH:O	2.53	0.41
1:E:7:GLU:HG2	1:E:11:GLY:HA3	2.03	0.40
1:D:109:ASN:HB3	1:D:259:TRP:CH2	2.56	0.40
1:E:7:GLU:CG	1:E:11:GLY:HA3	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:MET:HE1	1:B:174:LEU:HB2	2.03	0.40
1:D:104:GLY:HA3	1:D:105:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	347/361 (96%)	341 (98%)	6 (2%)	0	100	100
1	B	345/361 (96%)	339 (98%)	6 (2%)	0	100	100
1	C	337/361 (93%)	332 (98%)	5 (2%)	0	100	100
1	D	343/361 (95%)	335 (98%)	8 (2%)	0	100	100
1	E	343/361 (95%)	337 (98%)	6 (2%)	0	100	100
1	F	345/361 (96%)	339 (98%)	6 (2%)	0	100	100
All	All	2060/2166 (95%)	2023 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	281/292 (96%)	279 (99%)	2 (1%)	87	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	280/292 (96%)	278 (99%)	2 (1%)	87	84
1	C	271/292 (93%)	268 (99%)	3 (1%)	78	72
1	D	278/292 (95%)	276 (99%)	2 (1%)	87	84
1	E	278/292 (95%)	275 (99%)	3 (1%)	78	72
1	F	279/292 (96%)	278 (100%)	1 (0%)	93	91
All	All	1667/1752 (95%)	1654 (99%)	13 (1%)	85	81

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	55	TRP
1	B	33	LEU
1	B	55	TRP
1	C	55	TRP
1	C	197	SER
1	C	249	MET
1	D	42	LEU
1	D	55	TRP
1	E	55	TRP
1	E	130	GLU
1	E	244	ARG
1	F	55	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	65	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

40 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	EDO	A	401	-	3,3,3	0.50	0	2,2,2	0.35	0
2	EDO	A	402	-	3,3,3	0.53	0	2,2,2	0.37	0
2	EDO	A	403	-	3,3,3	0.54	0	2,2,2	0.25	0
2	EDO	A	404	-	3,3,3	0.41	0	2,2,2	0.43	0
2	EDO	A	405	-	3,3,3	0.69	0	2,2,2	0.32	0
2	EDO	A	406	-	3,3,3	0.69	0	2,2,2	0.49	0
2	EDO	A	407	-	3,3,3	0.46	0	2,2,2	0.37	0
3	GOL	A	408	-	5,5,5	0.32	0	5,5,5	0.43	0
4	ACT	A	409	-	1,3,3	0.62	0	0,3,3	0.00	-
2	EDO	B	401	-	3,3,3	0.45	0	2,2,2	0.43	0
2	EDO	B	402	-	3,3,3	0.46	0	2,2,2	0.37	0
2	EDO	B	403	-	3,3,3	0.37	0	2,2,2	0.85	0
2	EDO	B	404	-	3,3,3	0.51	0	2,2,2	0.31	0
2	EDO	B	405	-	3,3,3	0.42	0	2,2,2	0.37	0
4	ACT	B	406	-	1,3,3	0.96	0	0,3,3	0.00	-
2	EDO	C	401	-	3,3,3	0.48	0	2,2,2	0.35	0
2	EDO	C	402	-	3,3,3	0.33	0	2,2,2	0.71	0
2	EDO	C	403	-	3,3,3	0.58	0	2,2,2	0.32	0
2	EDO	C	404	-	3,3,3	0.37	0	2,2,2	0.47	0
2	EDO	C	405	-	3,3,3	0.51	0	2,2,2	0.36	0
2	EDO	C	406	-	3,3,3	0.56	0	2,2,2	0.31	0
3	GOL	C	407	-	5,5,5	0.29	0	5,5,5	0.22	0
3	GOL	C	408	-	5,5,5	0.38	0	5,5,5	0.47	0
4	ACT	C	409	-	1,3,3	1.32	0	0,3,3	0.00	-
2	EDO	D	401	-	3,3,3	0.50	0	2,2,2	0.83	0
2	EDO	D	402	-	3,3,3	0.47	0	2,2,2	0.26	0
2	EDO	D	403	-	3,3,3	0.49	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	D	404	-	5,5,5	0.29	0	5,5,5	0.47	0
3	GOL	D	405	-	5,5,5	0.28	0	5,5,5	0.33	0
4	ACT	D	406	-	1,3,3	0.87	0	0,3,3	0.00	-
2	EDO	E	401	-	3,3,3	0.46	0	2,2,2	0.50	0
2	EDO	E	402	-	3,3,3	0.45	0	2,2,2	0.43	0
4	ACT	E	403	-	1,3,3	1.79	0	0,3,3	0.00	-
4	ACT	E	404	-	1,3,3	1.90	0	0,3,3	0.00	-
2	EDO	F	401	-	3,3,3	0.52	0	2,2,2	0.43	0
2	EDO	F	402	-	3,3,3	0.47	0	2,2,2	0.35	0
3	GOL	F	403	-	5,5,5	0.39	0	5,5,5	0.62	0
3	GOL	F	404	-	5,5,5	0.24	0	5,5,5	0.38	0
3	GOL	F	405	-	5,5,5	0.33	0	5,5,5	0.16	0
4	ACT	F	406	-	1,3,3	0.63	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	401	-	-	0/1/1/1	0/0/0/0
2	EDO	A	402	-	-	0/1/1/1	0/0/0/0
2	EDO	A	403	-	-	0/1/1/1	0/0/0/0
2	EDO	A	404	-	-	0/1/1/1	0/0/0/0
2	EDO	A	405	-	-	0/1/1/1	0/0/0/0
2	EDO	A	406	-	-	0/1/1/1	0/0/0/0
2	EDO	A	407	-	-	0/1/1/1	0/0/0/0
3	GOL	A	408	-	-	0/4/4/4	0/0/0/0
4	ACT	A	409	-	-	0/0/0/0	0/0/0/0
2	EDO	B	401	-	-	0/1/1/1	0/0/0/0
2	EDO	B	402	-	-	0/1/1/1	0/0/0/0
2	EDO	B	403	-	-	0/1/1/1	0/0/0/0
2	EDO	B	404	-	-	0/1/1/1	0/0/0/0
2	EDO	B	405	-	-	0/1/1/1	0/0/0/0
4	ACT	B	406	-	-	0/0/0/0	0/0/0/0
2	EDO	C	401	-	-	0/1/1/1	0/0/0/0
2	EDO	C	402	-	-	0/1/1/1	0/0/0/0
2	EDO	C	403	-	-	0/1/1/1	0/0/0/0
2	EDO	C	404	-	-	0/1/1/1	0/0/0/0
2	EDO	C	405	-	-	0/1/1/1	0/0/0/0
2	EDO	C	406	-	-	0/1/1/1	0/0/0/0
3	GOL	C	407	-	-	0/4/4/4	0/0/0/0
3	GOL	C	408	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACT	C	409	-	-	0/0/0/0	0/0/0/0
2	EDO	D	401	-	-	0/1/1/1	0/0/0/0
2	EDO	D	402	-	-	0/1/1/1	0/0/0/0
2	EDO	D	403	-	-	0/1/1/1	0/0/0/0
3	GOL	D	404	-	-	0/4/4/4	0/0/0/0
3	GOL	D	405	-	-	0/4/4/4	0/0/0/0
4	ACT	D	406	-	-	0/0/0/0	0/0/0/0
2	EDO	E	401	-	-	0/1/1/1	0/0/0/0
2	EDO	E	402	-	-	0/1/1/1	0/0/0/0
4	ACT	E	403	-	-	0/0/0/0	0/0/0/0
4	ACT	E	404	-	-	0/0/0/0	0/0/0/0
2	EDO	F	401	-	-	0/1/1/1	0/0/0/0
2	EDO	F	402	-	-	0/1/1/1	0/0/0/0
3	GOL	F	403	-	-	0/4/4/4	0/0/0/0
3	GOL	F	404	-	-	0/4/4/4	0/0/0/0
3	GOL	F	405	-	-	0/4/4/4	0/0/0/0
4	ACT	F	406	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	403	EDO	2	0
2	A	405	EDO	1	0
3	A	408	GOL	1	0
2	B	405	EDO	3	0
2	C	403	EDO	2	0
2	C	404	EDO	4	0
3	C	408	GOL	2	0
2	D	401	EDO	5	0
2	D	402	EDO	2	0
3	D	405	GOL	1	0
4	E	403	ACT	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	347/361 (96%)	-0.59	3 (0%)	84	82	14, 23, 39, 57	0
1	B	345/361 (95%)	-0.47	2 (0%)	89	87	15, 25, 43, 64	0
1	C	339/361 (93%)	-0.51	2 (0%)	89	87	17, 27, 45, 67	0
1	D	345/361 (95%)	0.48	46 (13%)	4	2	17, 39, 67, 83	0
1	E	345/361 (95%)	0.35	36 (10%)	7	5	22, 39, 63, 83	0
1	F	347/361 (96%)	-0.52	0	100	100	13, 22, 37, 53	0
All	All	2068/2166 (95%)	-0.21	89 (4%)	36	30	13, 28, 57, 83	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	20	PRO	7.0
1	D	18	ILE	6.1
1	D	15	LEU	6.0
1	D	30	PRO	5.6
1	D	19	GLY	5.1
1	D	16	ILE	5.0
1	D	33	LEU	4.7
1	E	44	ALA	4.6
1	E	126	TYR	4.5
1	D	44	ALA	4.5
1	D	126	TYR	4.5
1	E	45	ASP	4.4
1	E	46	LYS	4.3
1	D	123	LEU	4.3
1	D	124	THR	4.1
1	E	3	SER	4.0
1	D	121	THR	4.0
1	D	8	GLU	4.0
1	E	12	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	128	GLY	3.9
1	E	8	GLU	3.9
1	D	3	SER	3.9
1	D	32	CYS	3.8
1	D	40	GLY	3.8
1	E	127	PHE	3.8
1	D	244	ARG	3.7
1	E	7	GLU	3.7
1	D	11	GLY	3.6
1	D	7	GLU	3.6
1	D	46	LYS	3.6
1	D	125	GLU	3.5
1	B	195	ARG	3.5
1	D	120	HIS	3.4
1	E	43	ASN	3.3
1	E	236	MET	3.3
1	D	122	LEU	3.3
1	D	45	ASP	3.2
1	D	127	PHE	3.2
1	D	2	ASN	3.2
1	D	36	VAL	3.2
1	D	310	ASN	3.1
1	E	6	THR	3.1
1	D	14	GLU	3.1
1	D	17	ASN	3.1
1	E	244	ARG	3.0
1	D	12	PRO	3.0
1	E	125	GLU	2.9
1	E	13	PHE	2.9
1	E	130	GLU	2.9
1	E	232	GLU	2.9
1	A	12	PRO	2.8
1	E	231	PHE	2.8
1	E	41	ALA	2.7
1	E	128	GLY	2.7
1	E	195	ARG	2.7
1	D	9	ASN	2.7
1	E	5	TYR	2.7
1	E	70	GLU	2.7
1	E	71	GLY	2.7
1	B	28	CYS	2.6
1	E	230	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	42	LEU	2.6
1	D	152	TYR	2.5
1	C	310	ASN	2.5
1	D	91	LEU	2.4
1	C	348	ALA	2.4
1	E	129	ILE	2.4
1	E	235	GLN	2.4
1	D	10	HIS	2.3
1	E	240	GLY	2.3
1	E	9	ASN	2.3
1	D	6	THR	2.3
1	D	22	PRO	2.3
1	D	232	GLU	2.3
1	E	42	LEU	2.3
1	E	11	GLY	2.2
1	D	236	MET	2.2
1	E	47	SER	2.2
1	A	310	ASN	2.1
1	D	29	MET	2.1
1	D	43	ASN	2.1
1	D	117	SER	2.1
1	E	40	GLY	2.1
1	E	14	GLU	2.1
1	E	39	HIS	2.1
1	A	8	GLU	2.0
1	E	4	TYR	2.0
1	D	282	LYS	2.0
1	D	31	GLU	2.0

6.2　Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3　Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4　Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	F	404	6/6	0.66	0.17	10.01	52,55,55,56	0
2	EDO	C	401	4/4	0.81	0.25	9.92	53,53,53,54	0
2	EDO	A	406	4/4	0.79	0.18	8.95	37,40,41,42	0
2	EDO	B	404	4/4	0.60	0.22	7.73	58,59,59,59	0
2	EDO	A	403	4/4	0.68	0.22	7.71	51,53,56,56	0
2	EDO	A	405	4/4	0.79	0.15	7.24	37,42,44,47	0
2	EDO	D	403	4/4	0.80	0.18	6.59	51,54,55,57	0
2	EDO	C	403	4/4	0.88	0.12	5.30	38,40,40,40	0
2	EDO	C	404	4/4	0.90	0.15	4.86	44,47,49,51	0
3	GOL	C	408	6/6	0.67	0.18	4.43	50,54,56,57	0
2	EDO	C	402	4/4	0.91	0.16	4.41	39,45,49,51	0
2	EDO	C	406	4/4	0.70	0.19	4.36	52,53,53,54	0
2	EDO	A	407	4/4	0.94	0.12	4.00	26,34,38,39	0
4	ACT	D	406	4/4	0.93	0.14	3.78	30,31,31,35	0
2	EDO	E	402	4/4	0.92	0.12	3.64	54,56,58,59	0
3	GOL	A	408	6/6	0.79	0.15	3.45	50,50,51,52	0
4	ACT	E	404	4/4	0.58	0.22	3.34	43,45,47,47	0
4	ACT	C	409	4/4	0.95	0.09	3.25	27,30,31,32	0
3	GOL	F	405	6/6	0.85	0.10	3.02	54,54,55,56	0
2	EDO	B	403	4/4	0.87	0.14	2.90	43,43,43,47	0
3	GOL	F	403	6/6	0.91	0.12	2.89	34,43,46,47	0
2	EDO	F	401	4/4	0.85	0.15	2.68	40,44,44,45	0
2	EDO	A	401	4/4	0.87	0.16	2.16	48,50,51,51	0
3	GOL	D	404	6/6	0.85	0.11	1.87	64,66,67,69	0
2	EDO	D	401	4/4	0.94	0.11	1.60	28,29,30,37	0
3	GOL	C	407	6/6	0.90	0.13	1.58	57,57,57,57	0
4	ACT	A	409	4/4	0.95	0.08	1.55	23,25,26,27	0
4	ACT	E	403	4/4	0.89	0.14	1.41	33,33,37,40	0
2	EDO	A	404	4/4	0.88	0.12	0.89	37,38,41,42	0
3	GOL	D	405	6/6	0.88	0.12	0.79	45,53,54,54	0
4	ACT	F	406	4/4	0.90	0.10	0.78	24,25,27,27	0
2	EDO	E	401	4/4	0.90	0.12	0.67	39,43,45,46	0
2	EDO	A	402	4/4	0.82	0.13	0.65	49,49,49,50	0
4	ACT	B	406	4/4	0.93	0.09	-0.02	26,26,29,31	0
2	EDO	C	405	4/4	0.85	0.09	-0.33	55,55,55,56	0
2	EDO	F	402	4/4	0.95	0.09	-0.38	52,53,55,55	0
2	EDO	B	402	4/4	0.85	0.09	-0.52	55,55,56,56	0
2	EDO	B	401	4/4	0.92	0.11	-	56,56,56,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	EDO	B	405	4/4	0.56	0.17	-	70,70,71,71	0
2	EDO	D	402	4/4	0.75	0.14	-	57,59,59,59	0

6.5 Other polymers ⓘ

There are no such residues in this entry.